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Minimization Search Method For Data Inversion

In the physical, biological, or social sciences, an experimenter often makes a series of measurements of a dependent variable as correspond to values of a selected subset of the independent variables occurring in a known mathematical formulation. For instance, if $X = f(a, b, c, d)$, measurements of X might be made at a selected value of a and at $b = b_1, b_2, b_3, \dots$ etc. The remaining unknowns, independent variables c and d , may be of primary interest, but their values cannot generally be determined analytically from the known relationship. Instead, one must take successive guesses for c and d , until values of c and d are found that give a value of X sufficiently close to the measured X (at all the values of b for which measurements are taken).

Several methods, such as least-squares techniques, are known for finding the values of such variables. However, the required computation time using a new technique, the minimization search method, increases with the 1st power of the number of variables. This is in contrast with classical minimization methods for which the computational time increases with the 3d power of the number of variables.

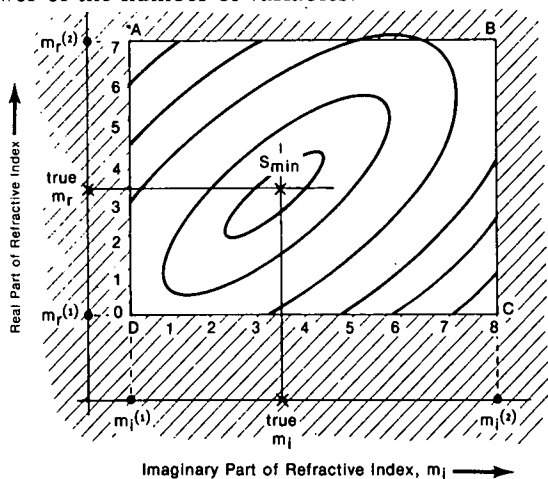


Figure 1. Meaningful Values of m_i and m_r .
The "Contour Lines" Represent Lines
of Equal Value of the Function S .

The new method was developed to calculate refractive indices from measurements taken by a spectrometer described in NASA Tech Brief B75-10335. In that case it was desired to determine the values of the independent real and complex terms of the refractive index (m_r and m_i) which are related to a series of measurable quantities I_q (intensities):

$$I_q \equiv I(s_q; m_r, m_i)$$

where s_q represents one or more independent variables with known values. The problem is to find for any and all q the particular couple (m_r, m_i) such that $|\bar{I}_q - I_q| \leq \epsilon_q$, where \bar{I}_q is the observed value, I_q is the calculated value, and ϵ_q is the upper bound for accuracy. (The values ϵ_q can be different for each q .)

To find the values of m_i and m_r , a surface is defined

$$S(s_q; m_r, m_i) = \sum_q \left[\frac{\bar{I}_q - I_q}{d_q I_q} \right]^2 \quad (1)$$

where d_q is a statistical weighting factor related to the manner in which the values of s_q (at which measurements are taken) are chosen and to the weights accorded the individual measurements \bar{I}_q . Such a surface is shown in Figure 1. The minimum of the surface S_{min} , corresponds to the values of m_i and m_r within the required accuracy. The minimization search method can be used to find the point.

The first step is to apply any physical or theoretical information which limits the range of values for the minimum. In Figure 1 the rectangle ABCD represents the region of possible physically meaningful values of m_i and m_r . Then an initial guess, $m_r^{(0)}$ and $m_i^{(0)}$, is made and defines point 0 that serves as an "origin"

(continued overleaf)



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